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Theoretical and numerical studies of the positions of cold trapped ions

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Abstract

We examine the properties of cold ions confined by a Paul trap in a linear crystal configuration, a system of considerable current interest due to its application to practical quantum computation. Using a combination of theoretical and numerical calculations, a semi-empirical formula for the positions of the ions is derived. © 1998 Published by Elsevier Science B.V.

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Cold ions confined in electromagnetic traps are rapidly becoming a very important system both for the study of fundamental physical systems, such as cold charged plasmas or quantum chaos, and for technological applications such as optical frequency standards. Recently a chain of cold ions in a linear trap has been proposed as a possible means to realize a quantum computer [1]. This idea was confirmed in principal soon after when an elementary quantum logic gate was realized experimentally using a trapped Beryllium ion [2], and larger scale devices are currently being pursued by several experimental groups (see, for example, Ref. [3]). Understanding the properties of collections of confined ions is of great importance to these endeavors.

As is well known [4], it is impossible to confine charged particles by electrostatic forces alone. To overcome this problem, the radio-frequency Paul trap was developed: such devices use a electromagnetic field varying at radio frequencies ($\sim$100 MHz say) to produce an *effective* binding potential in three dimensions [5]. When two or more ions are confined in such a trap, they will repel each other due to the Coulomb force. As a result, such confined charged plasmas will have very low densities. When sufficiently cold, the plasma will condense into a crystalline state. In the highly anisotropic traps used for some atomic clocks [6] and for quantum computing, this crystalline state is, for small enough numbers of ions, a simple chain of ions lying in a straight line. As the degree of anisotropy is decreased, or number of ions is increased, phase changes to other configurations will occur: firstly the ions adopt a zig-zag configuration, and then a helical

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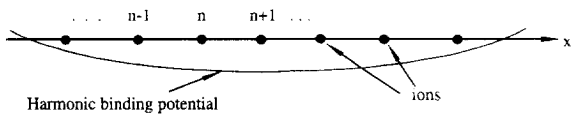

Fig. 1. A schematic illustration of ions confined in an harmonic trapping potential.

configuration. These phase changes have been studies numerically [7] and analytically [8].

In this Letter we present results of new numerical studies of the positions of ions confined in highly anisotropic traps. This information is of course of considerable importance in designing trapped ion quantum computers. Using a simple theoretical argument we then develop a relatively compact expression for the position of each ion, which depends on the total number of ions confined in the chain. Our results are compared with both our numerical data, and with results obtained previously by other authors, and good agreement is obtained.

Consider a chain of N ions confined in a linear trap (Fig.1). The position of the nth ion, where the ions are numbered from left to right, will be denoted by the position vector relative to the trap center (i.e. the minimum of the binding potential) $\boldsymbol{R}_n(t) = (X_n(t), Y_n(t), Z_n(t))$. The motion of each ion will be influenced by an overall harmonic potential due to the trap electrodes, and by the Coulomb force exerted by all of the other ions. Thus the potential energy of the ions in the ion chain is given by the following expression,

$$V(\boldsymbol{R}_1, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N) = \frac{M}{2}\sum_{n=1}^{N}(\omega_x^2 X_n^2 + \omega_y^2 Y_n^2 + \omega_z^2 Z_n^2) + \frac{e^2}{8\pi\epsilon_0}\sum_{\substack{n,m=1 \\ m\neq n}}^{N}\frac{1}{|\boldsymbol{R}_n - \boldsymbol{R}_m|}, \tag{1}$$

where M is the mass of each ion, e is the electron charge (the ions are assumed to be singly ionized), ϵ_0 is the permittivity of free space and ω_x is the angular frequency characterizing the strength of the trapping potential in the x direction (and similarly ω_y and ω_z for the y and z directions).

The equilibrium positions of the ions, $\boldsymbol{R}_m^{(0)}$, are defined by solutions of the following equations,

$$[\nabla V(\boldsymbol{R}_1, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N)]_{\boldsymbol{R}_m = \boldsymbol{R}_m^{(0)}} = 0. \tag{2}$$

Substituting from (1) we obtain

$$M\omega_i^2 X_m^{i(0)} - \frac{e^2}{4\pi\epsilon_0}\sum_{\substack{n=1 \\ m\neq n}}^{N}\frac{X_n^{i(0)} - X_m^{i(0)}}{|\boldsymbol{R}_n^{(0)} - \boldsymbol{R}_m^{(0)}|^3} = 0 \quad (i = 1,2,3), \tag{3}$$

where $i = (1,2,3)$ denote the X, Y and Z components, respectively.

Let us assume that the trap potentials are sufficiently strong in the Y and Z directions and sufficiently weak in the X direction that in equilibrium the ions lie in a straight line along the X-axis. Mathematically this assumption is expressed by

$$\boldsymbol{R}_n^{(0)} = \ell(u_n, 0, 0), \tag{4}$$

where ℓ is a scale length given by $(e^2/4\pi\epsilon_0 M\omega_x^2)^{1/3}$ and u_n is the dimensionless equilibrium position of the nth ion, which is a solution of the following set of N coupled algebraic equations, obtained by substitution from Eq. (4) into Eq. (3),

$$u_m + \sum_{\substack{n=1 \\ m\neq n}}^{N}\frac{\mathrm{sgn}(u_m - u_n)}{(u_m - u_n)^2} = 0 \quad (m = 1,2,\ldots,N), \tag{5}$$

where $\mathrm{sgn}(x) = 1$ if $x > 0$ and -1 if $x < 0$. For $N = 2$ and $N = 3$ these equations may be solved analytically [9]:

$$N = 2: \quad u_1 = -(1/2)^{2/3}, \quad u_2 = (1/2)^{2/3}, \tag{6}$$

$$N = 3: \quad u_1 = -(5/4)^{1/3}, u_2 = 0, \quad u_3 = (5/4)^{1/3}. \tag{7}$$

For $N > 2$ it is necessary to solve for the values of u_m numerically. For small numbers of ions ($N \leqslant 100$ say) a Newton–Raphson method can be employed to find u_m; however this becomes inefficient as N gets large. Therefore we used another method, based on the following set of equations of motion,

$$\ddot{v}_m(\tau) + \dot{v}_m(\tau) + v_m(\tau) + \sum_{\substack{n=1 \\ m \neq n}}^{N} \frac{\operatorname{sgn}(v_m(\tau) - v_n(\tau))}{(v_m(\tau) - v_n(\tau))^2} = 0 \quad (m = 1, 2, \ldots N), \tag{8}$$

where the single and double dots denote single and double differentiation with respect to the dimensionless time variable $\tau = \omega_x t$. These equations represent a hypothetical damped oscillation of the ions in the trap, including their mutual Coulomb interaction. The solutions of these equations have the property that

$$\lim_{\tau \to \infty} v_m(\tau) = u_m, \tag{9}$$

where u_m are the desired solutions of Eq. (5). The integration of Eq. (8) was carried out numerically using the standard fourth-order Runge-Kutta method [10]. Because Eq. (9) is valid regardless of the initial conditions, the simplest possible initial conditions were used, i.e. all of the ions being equally spaced. The Runge-Kutta algorithm was applied repeatedly until the values of u_m between adjacent iterations were identical to the seventh decimal place. This was done for up to 1000 ions (although not for all numbers). The values there by obtained are in agreement with those obtained (for $N \leqslant 100$) by the Newton–Raphson method [9]. This dynamic technique can be adapted quite easily to study classical wave motion in the ion chain; this will be the subject of a forthcoming paper.

In order to make some sense of the large amount of data generated [1], we will now derive a analytic formula which approximates the numerical results quite closely. Our analysis is based on the very elegant idea due to Garg [11]. Let us consider the force acting on an ion at position X. The Coulomb force due to the two nearest neighbor ions is

$$F_{\mathrm{nn}} = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{S_-^2} - \frac{1}{S_+^2}\right) \approx \frac{e^2}{4\pi\epsilon_0}\frac{2}{S(X)^2}\frac{\mathrm{d}S(X)}{\mathrm{d}X}, \tag{10}$$

where S_- is the distance from the ion to the nearest neighbor on the left, S_+ is the distance to the nearest neighbor on the right and $S(X)$ is the separation of ions at position X, treated as a continuous function. This is a reasonable approximation to make for large numbers of ions. The next nearest neighbors are approximately twice as far away as the nearest neighbors, and so the force they exert on the ion is approximately $F_{\mathrm{nn}}/4$; the next pair of ions are three times as far away as the nearest neighbors, and so the force they exert is approximately $F_{\mathrm{nn}}/9$, and so on. Thus the total Coulomb force on the ion will approximately be given by the following expression,

$$F_C \approx F_{\mathrm{nn}} \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{e^2}{4\pi\epsilon_0}\frac{\pi^2}{3S(X)^2}\frac{\mathrm{d}S(X)}{\mathrm{d}X}, \tag{11}$$

where we have used the fact that $\sum_{k=1}^{\infty} 1/k^2 = \pi^2/6$ and we have approximated the finite sum over all ions as an infinite sum. This approximation should be valid near the center of the ion chain, but will not yield very good results at the ends of the chain.

The Coulomb force acting on the ion at position X will be balanced by the harmonic restoring force due to the trap electrodes. Thus we can write the following identity,

$$\frac{e^2}{4\pi\epsilon_0}\frac{\pi^2}{3S(X)^2}\frac{\mathrm{d}S(X)}{\mathrm{d}X} - M\omega_x^2 X = 0. \tag{12}$$

If we introduce the dimensionless ion separation $\sigma(u) = S(X)/\ell$ and dimensionless distance from the trap center $u = X/\ell$, where, as before $\ell = (e^2/4\pi\epsilon_0 M\omega_x^2)^{1/3}$, we obtain the following differential equation for the separation,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}u} = \frac{3}{\pi^2}u\sigma^2. \tag{13}$$

This can be solved quite easily, yielding the formula [11]

$$\sigma(u) = \frac{2\pi^2/3}{C - u^2}, \tag{14}$$

where C is a constant, which could be determined from the value of the separation of ions at the trap center ($u = 0$).

[1] A data file called ion_positions.dat which contains the results of these numerical calculations can be found in the directory pub/james/Ion_Position_Data which can be accessed via anonymous ftp to t4.lanl.gov.

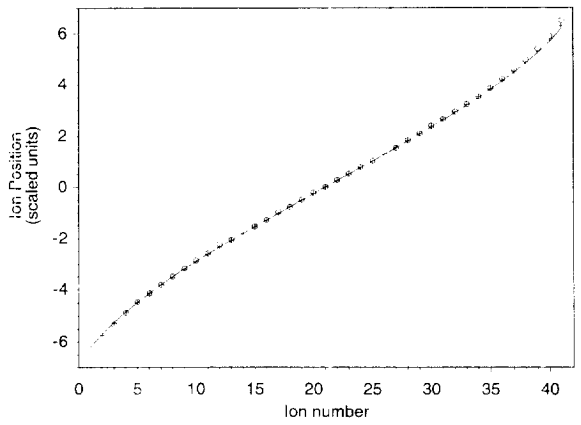

Fig. 2. Equilibrium positions of ions when there is a total of 41 in the chain, as calculated numerically (crosses) and by Eq. (18) (plane line). Also show are the experimental positions of Hg+ ions in a linear trap, which were gleaned from Fig. 5 of Ref. [6] (circles).

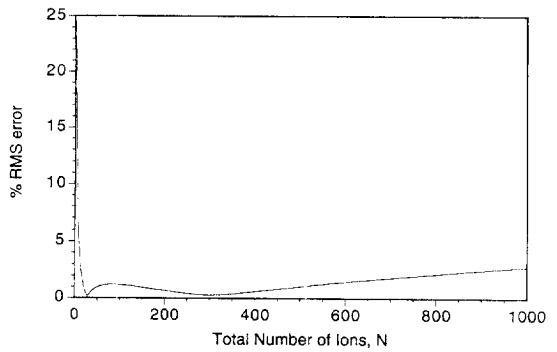

Fig. 3. Root mean square percentage error for calculating positions of trapped ions using formula Eq. (18) for total ion numbers N up to 1000.

Let $n(u)$ be the total number of ions which are within a scaled distance u of the trap center. Clearly $n(u)$ is given by the following differential equation,

$$\frac{\mathrm{d}n(u)}{\mathrm{d}u} = \frac{1}{\sigma(u)}. \tag{15}$$

On substitution from Eq. (14), and performing the integration, we obtain the following formula for $n(u)$,

$$n(u) = Au - Bu^3, \tag{16}$$

where we have set $n(0) = 0$. The constants A and B can be related to the constant C introduced above. However, instead of attempting to carry this analysis too far, it is better at this stage to obtain empirical formulas for the the constants A and B based on our numerical results. This was done by performing a least squares fit of the numerical data to a cubic formula of the type given by Eq. (16). The values of A and B were found for a variety of different total numbers of ions. When this data was compiled, we found that A and B were approximately given by the following power laws,

$$A(N) \approx 0.436N^{0.596},$$
$$B(N) \approx 0.0375N^{-0.178}, \tag{17}$$

where N is the total number of ions in the chain.

To obtain an expression for the position of the nth ion in the trap, it is necessary to invert Eq. (16). This can be done using the standard formulas for the roots of a cubic equation [12]. We therefore obtain, taking care to select the correct root based on the value of n at $u = 0$, the following formula for the the scaled equilibrium positions of the nth ion,

$$u_n = \sqrt{\frac{4A}{3B}} \cos\left\{\tfrac{1}{3}\cos^{-1}\left[-\sqrt{\frac{27B}{4A^3}} \times \left(n - \frac{N+1}{2}\right)\right] + \frac{4\pi}{3}\right\}$$
$$= \alpha(N)\sin\left(\tfrac{1}{3}\sin^{-1}\{\beta(N)[n-(N+1)/2]\}\right). \tag{18}$$

If we reintroduce the scale length ℓ, we finally obtain the following expression for the equilibrium position of the nth ion, when there are a total of N ions in the trap,

$$X_n^{(0)} = \left(\frac{e^2}{4\pi\epsilon_0 M\omega_x^2}\right)^{1/3} \alpha(N) \times \sin\left(\tfrac{1}{3}\sin^{-1}\{\beta(N)[n-(N+1)/2]\}\right), \tag{19}$$

where, as before, the ions are numbered from left to right, M is the mass of each ion, e is the electron charge, ϵ_0 is the permittivity of free space and ω_x is the angular frequency characterizing the strength of the trapping potential in the x direction. In Eqs. (18) and (19) we have introduced the coefficients $\alpha(N) = \sqrt{4A/3B} \approx 3.94N^{0.387}$ and $\beta(N) = \sqrt{27B/4A^3} \approx 1.75N^{-0.982}$.

Eq. (19) is the main result of this note. As an example we have plotted in Fig. 2 the numerically cal-

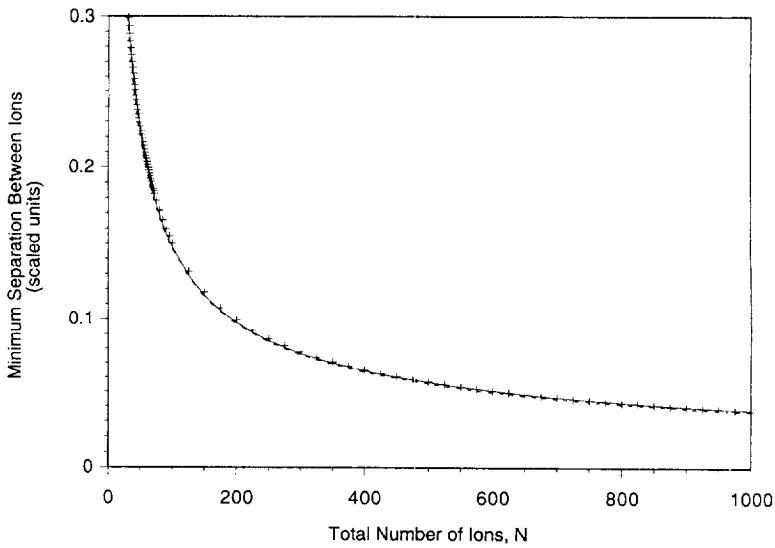

Fig. 4. Comparison of numerical results for minimum ion separations (crosses) with the empirical power law Eq. (21) (plane line) and the analytic formula Eq. (22) (dashed line). The two curves are in such good agreement that it is difficult to distinguish them.

culated ion positions together with the positions calculated using this formula, for a total of 41 ions in the trap. Also we have included experimental ion position data gleaned from Fig. 5 of Ref. [6]. As can be seen from the figure, there is good agreement between the numerical data and the empirical formula. The differences between the experimental data and that calculated numerically, may well be due to the departure of the trapping potential from the harmonic form we have assumed. The percentage r.m.s. error between the ion positions calculated numerically and those calculated using Eq. (18) is shown in Fig. 3. The error is only of the order of a few percent when $N > 25$, but as expected, errors increase for small numbers of ions.

For small arguments one can make the approximation $\sin(\sin^{-1}(x)/3) \approx x/3$, and so, near the trap center (where $n - N + 1/2$ is a small number) the scaled ion positions are given by

$$u_n \approx 2.29(n - N + 1/2)N^{-0.596}. \tag{20}$$

Hence the *minimum* separation between ions, which is of considerable importance in quantum computer design [13], is given by

$$u_{min}(N) \approx 2.29N^{-0.596}. \tag{21}$$

This result is in good agreement with the empirical formulas previously calculated for the minimum separation of ions are the trap center [13,14]. This formula is plotted in Fig. 4, along with the numerical data, and the following formula for the minimum ion spacing due to Dubin [8] (see also Ref. [11]), based on a fluid model for the ion cloud,

$$u_{min}(N) \approx 1.92N^{-2/3}\ln(aN)^{1/3}, \tag{22}$$

where $a = 6e^{\gamma - 13/5} \approx 0.794$, γ being Euler's constant. As can been seen from Fig. 4, both the empirical formula derived here and the analytic formula due to Dubin approximate the numerical data quite closely.

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